

FIG. 1

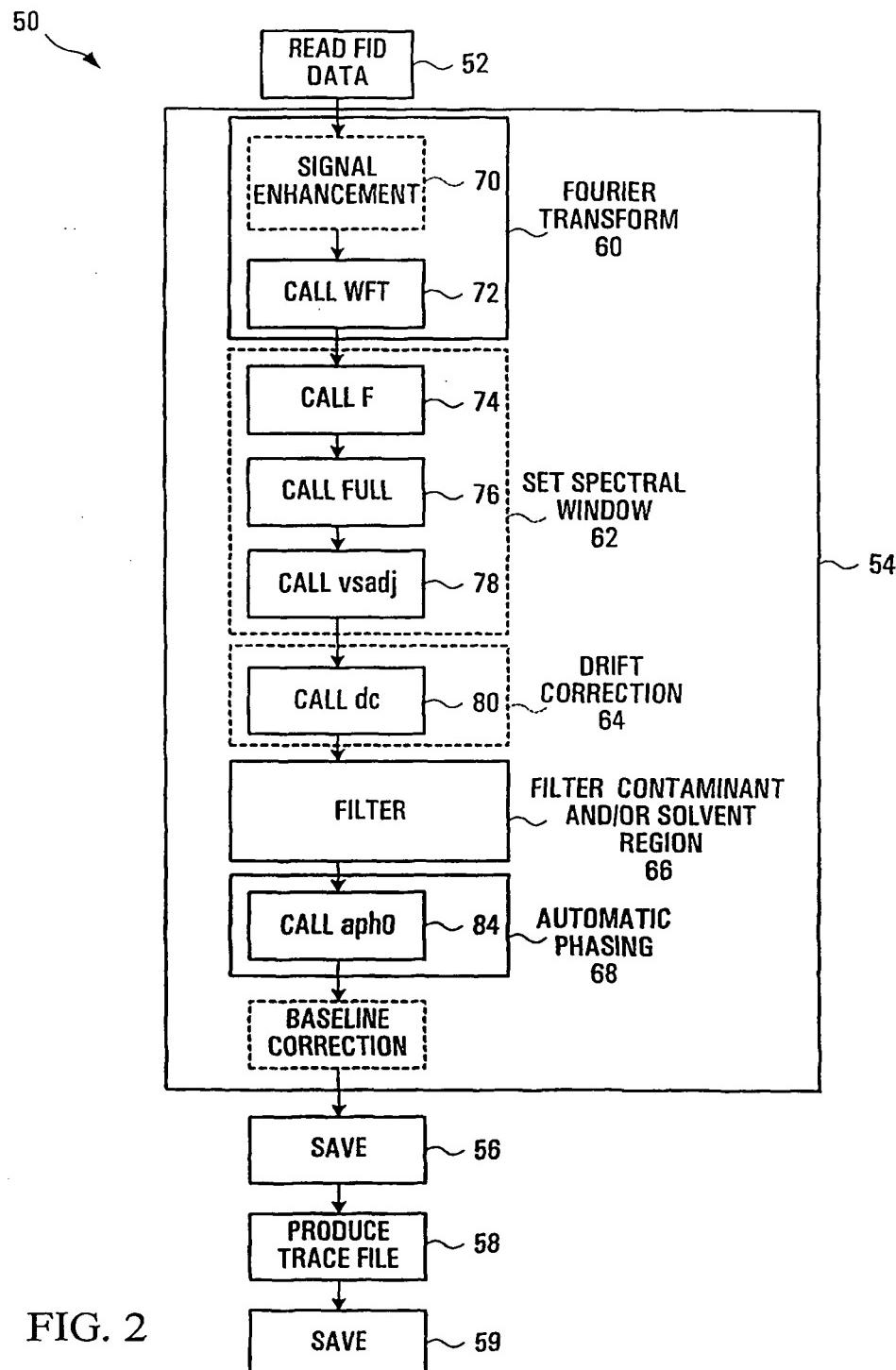
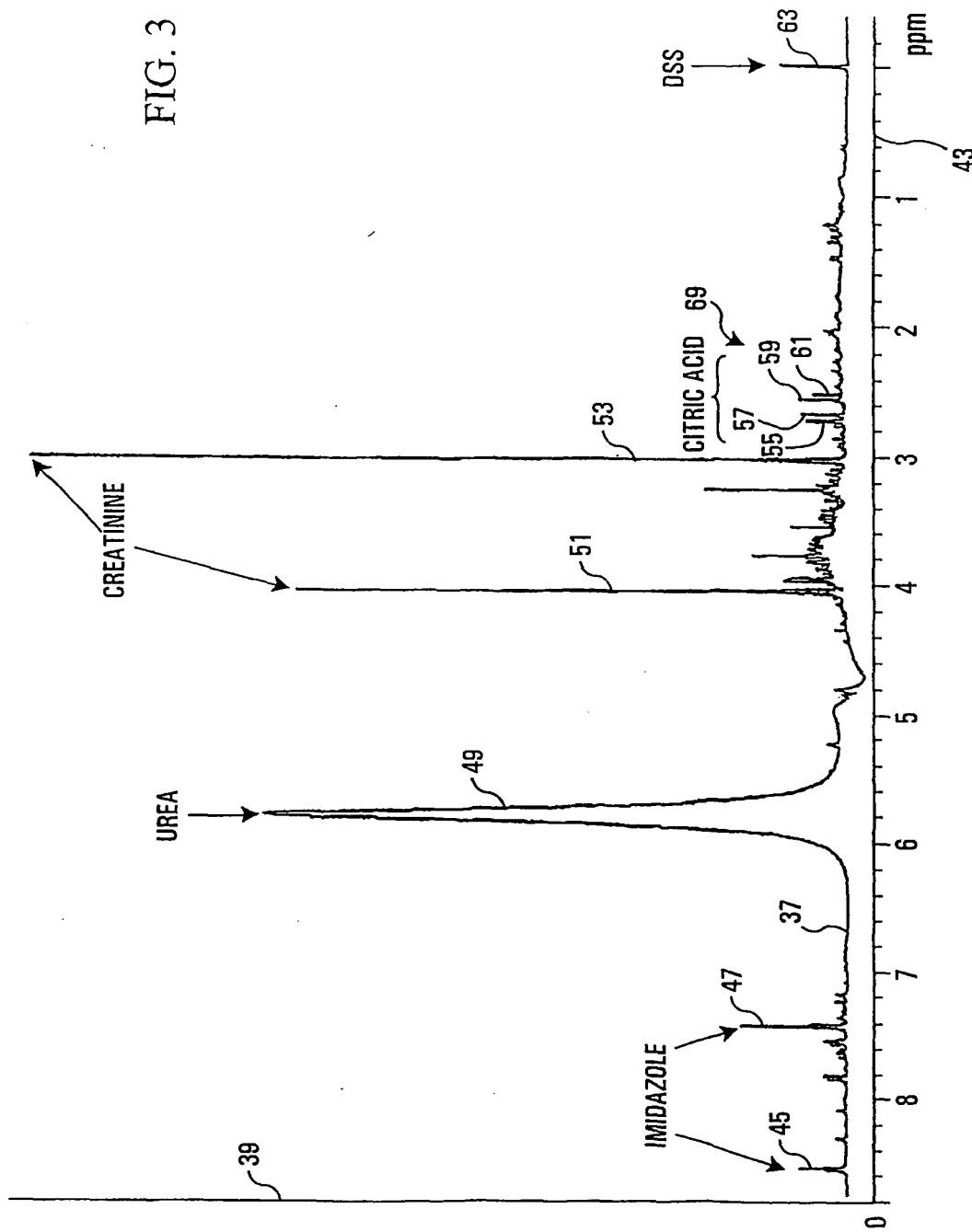


FIG. 2

FIG. 3



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FILTER SELECTED REGION

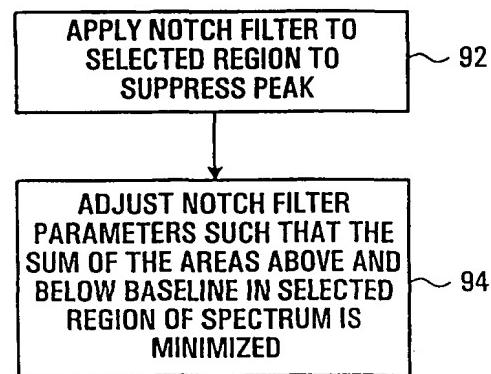


FIG. 4

**PROCESS FOR IDENTIFYING
COMPOUNDS FROM A TEST
SPECTRUM**

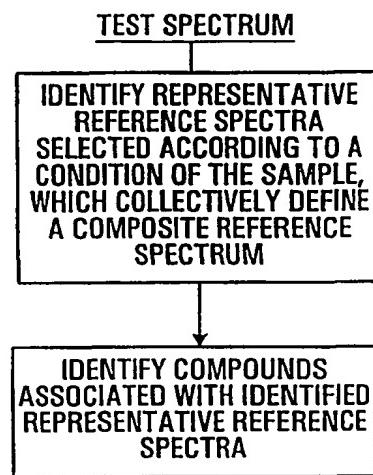
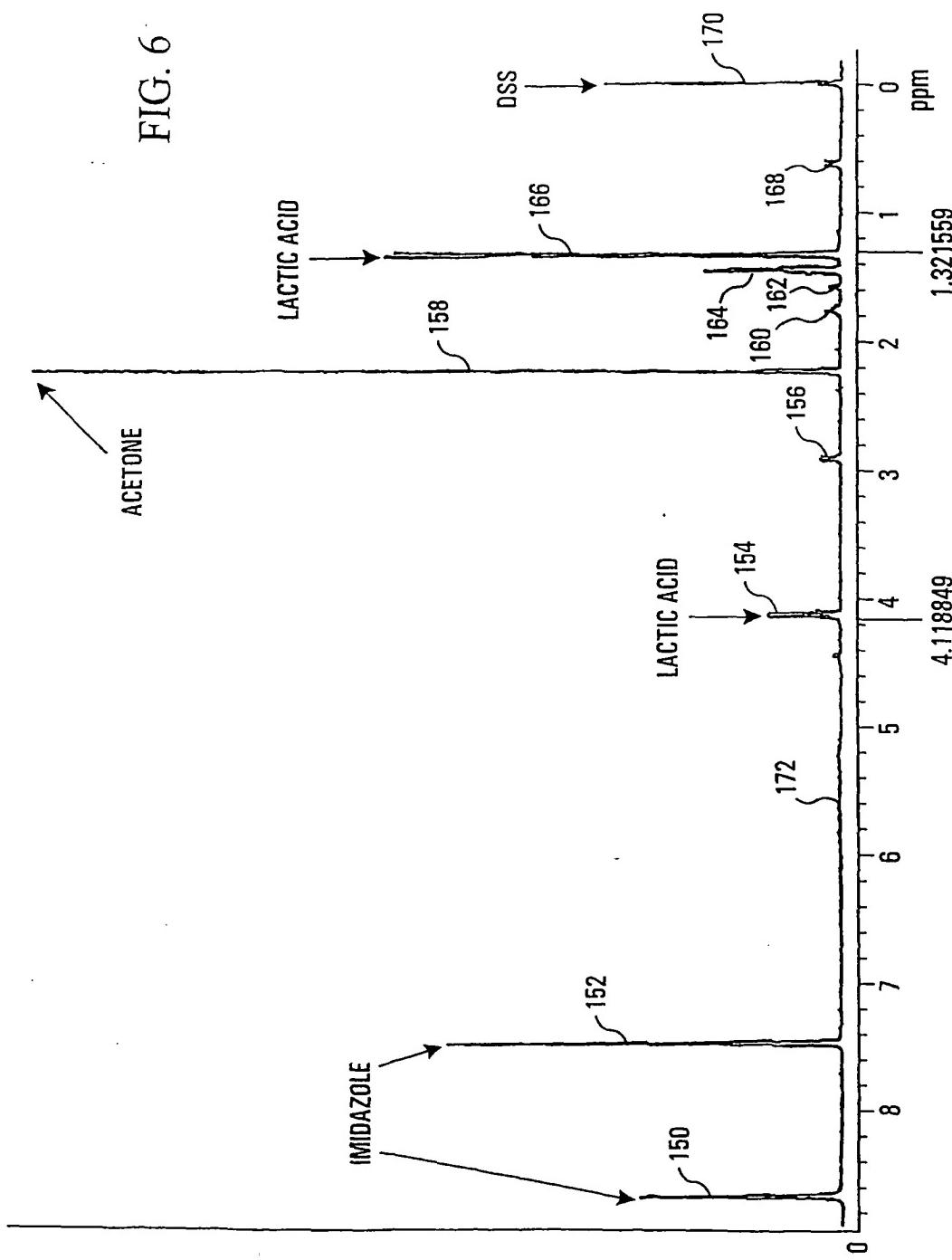


FIG. 5

FIG. 6



REAL SPECTRAL DATA · pH=5.10

```
< ?xml version="1.0"?>
<!-compoundDB version="2.0"->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>
```

200

```
<experiment>
  <pH>5.1</pH>
  <temperatureKelvin>298.150000</temperatureKelvin>
  <DSSRatio>0.533668</DSSRatio>
  <concentration>4.308710</concentration>
  <timestamp>Sept 5 2001</timestamp>
  <sourceFID>lacticacid.fid</sourceFID>
  <magnetMHz>400.120773</magnetMHz>
  <spectralWidthHz>6006.006006</spectralWidthHz>
</experiment>
```

202

```
<cluster>
  210  <protonNumber>3</protonNumber>  206
  212  <quantification>1</quantification>
  212  <subCluster>
    <centerPPM>1.321559</centerPPM>
  214  <lorentzianWidthAdjust>2.893258</lorentzianWidthAdjust>
  214  <peak>
    220  <offsetCenterHz>-3.455480</offsetCenterHz>
    222  <height>0.988680</height>
    224  <protonRatio>1.491461</protonRatio>
    224  </peak>
    224  <peak>
      220  <offsetCenterHz>3.455480</offsetCenterHz>
      222  <height>1.0000000</height>
      224  <protonRatio>1.508539</protonRatio>
      224  </peak>
    </subCluster>
</cluster>
```

204

FIG. 7A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> 4.118849 </centerPPM>
<lorentzianWidthAdjust> 13.441432 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.366999 </offsetCenterHz>
<height> 0.057244 </height>
<protonRatio> 0.130861 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.43221144 </offsetCenterHz>
<height> 0.164751 </height>
<protonRatio> 0.376629 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.487744 </offsetCenterHz>
<height> 0.161840 </height>
<protonRatio> 0.369975 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.366999 </offsetCenterHz>
<height> 0.053601 </height>
<protonRatio> 0.122535 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

208

204

FIG. 7B

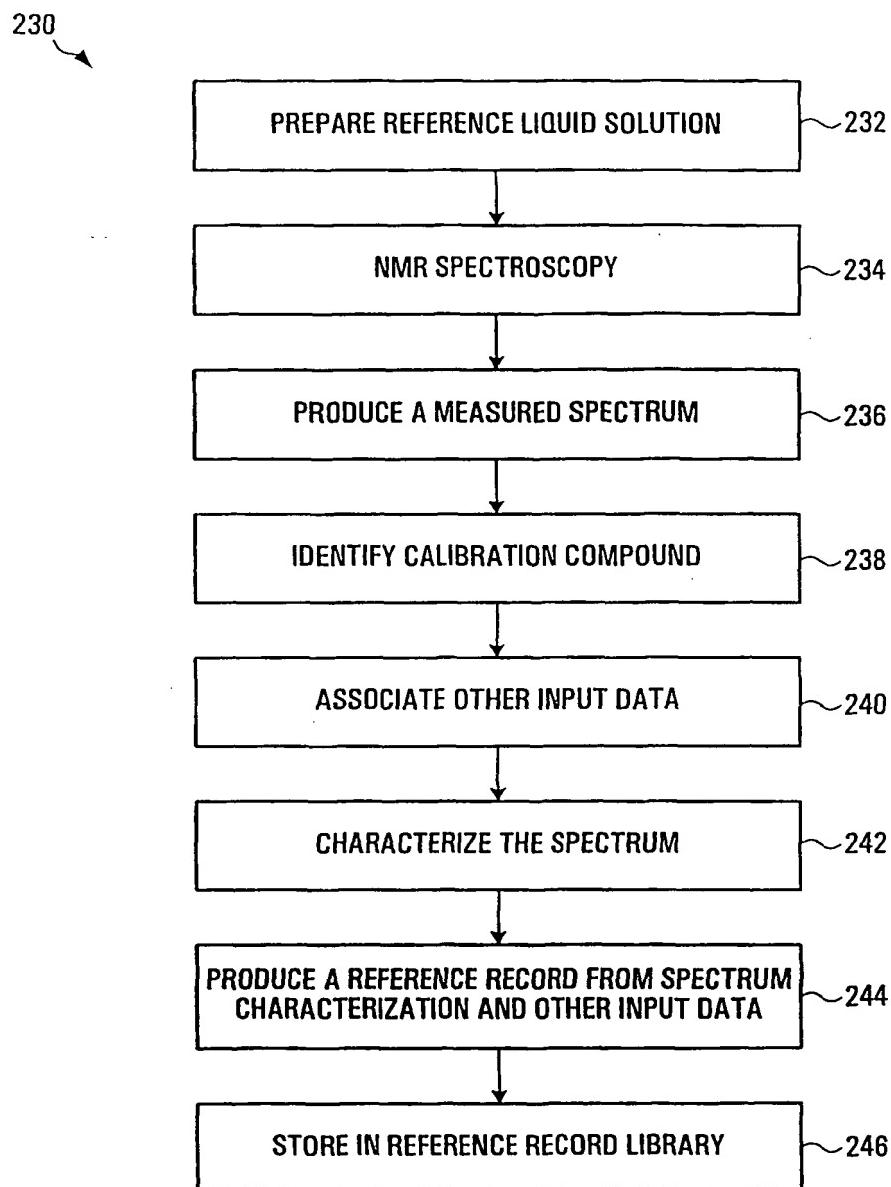


FIG. 8

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REFERENCE DETERMINATION

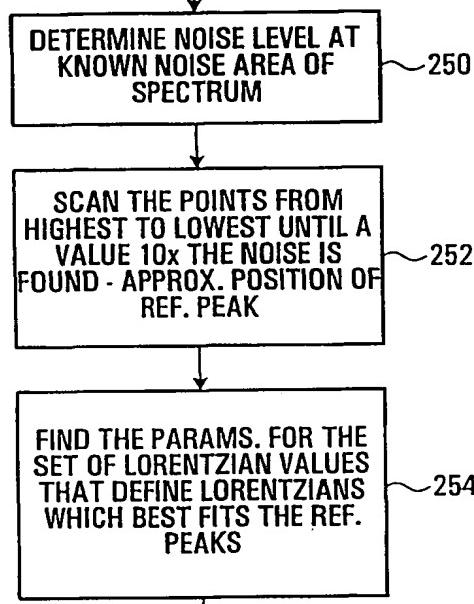


FIG. 9

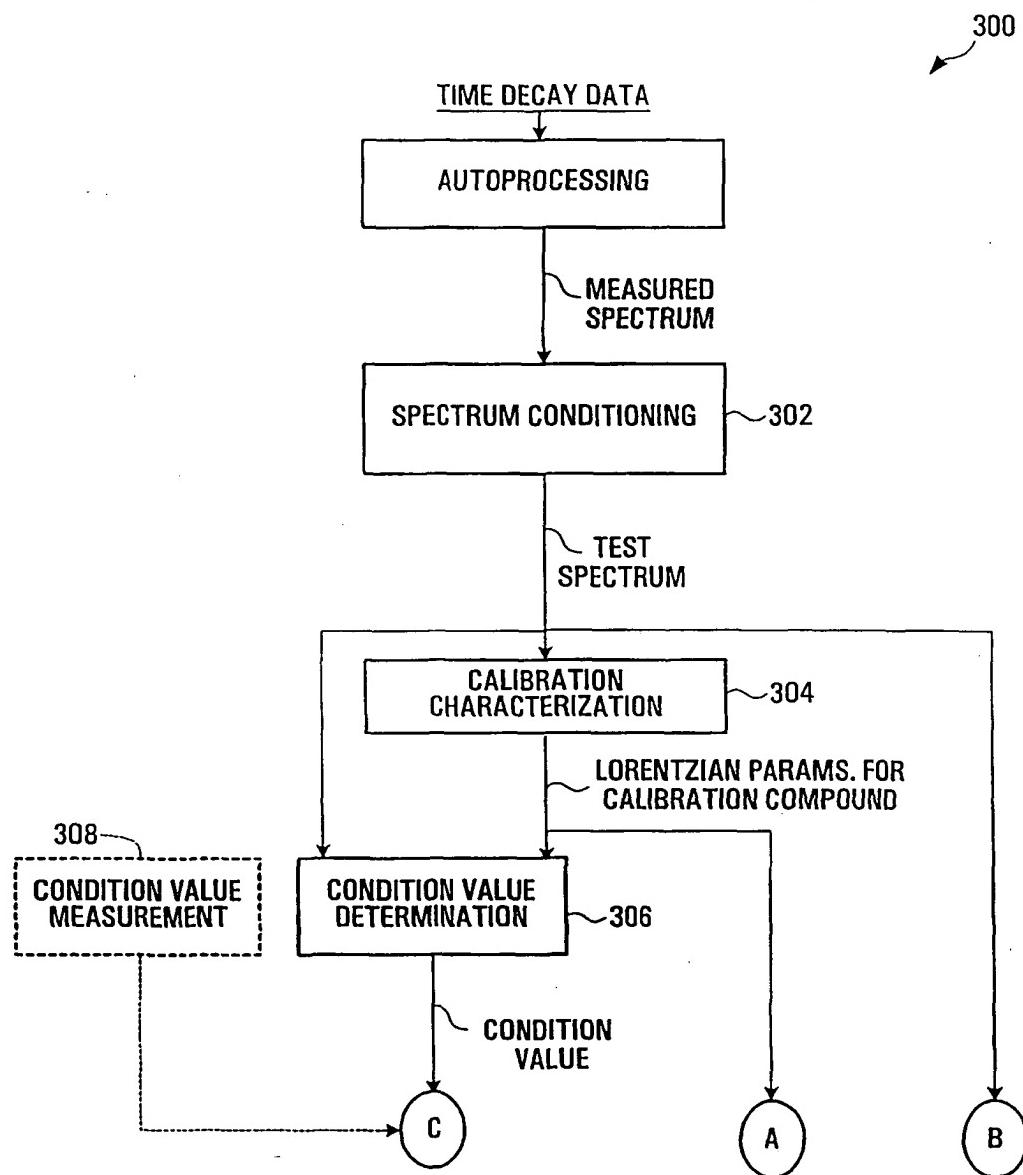


FIG. 10A

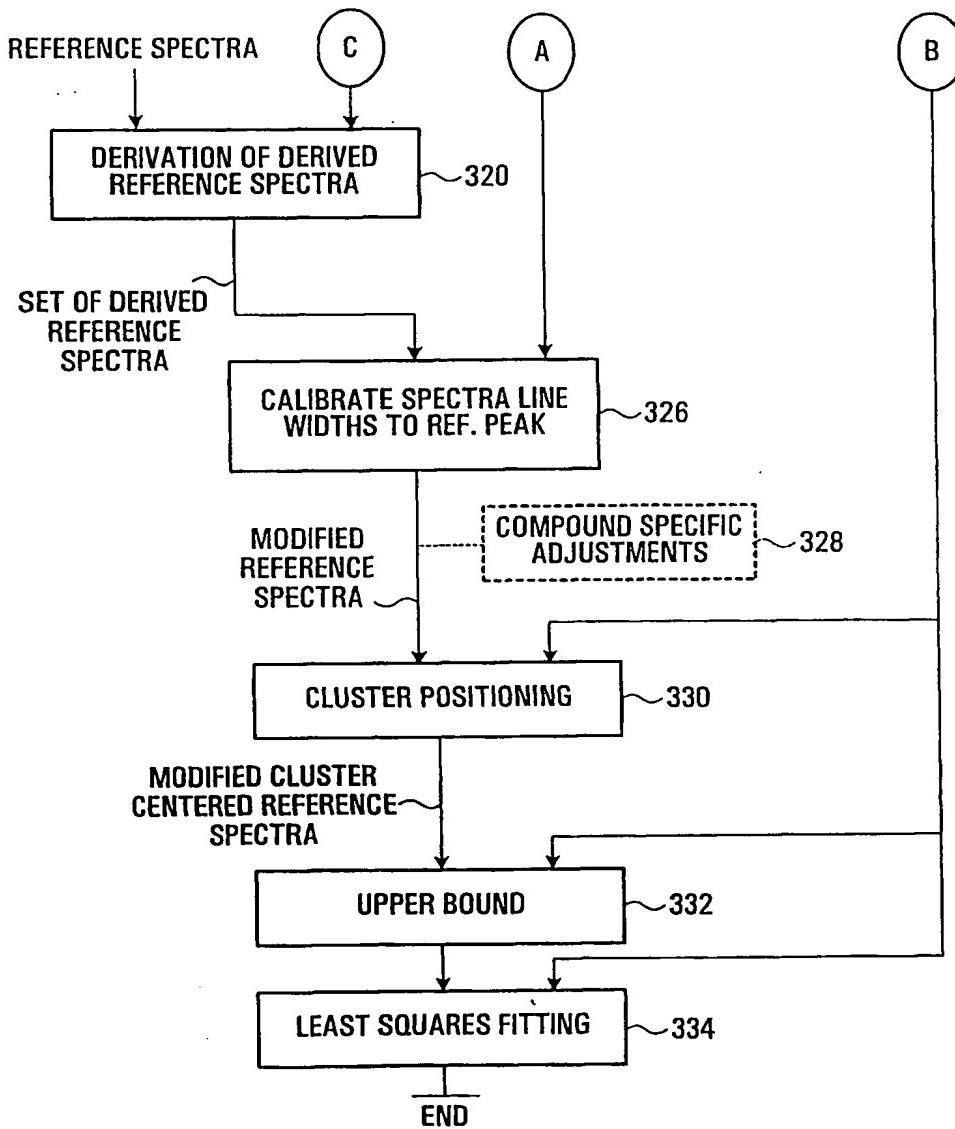


FIG. 10B

CONDITION VALUE DETERMINATION

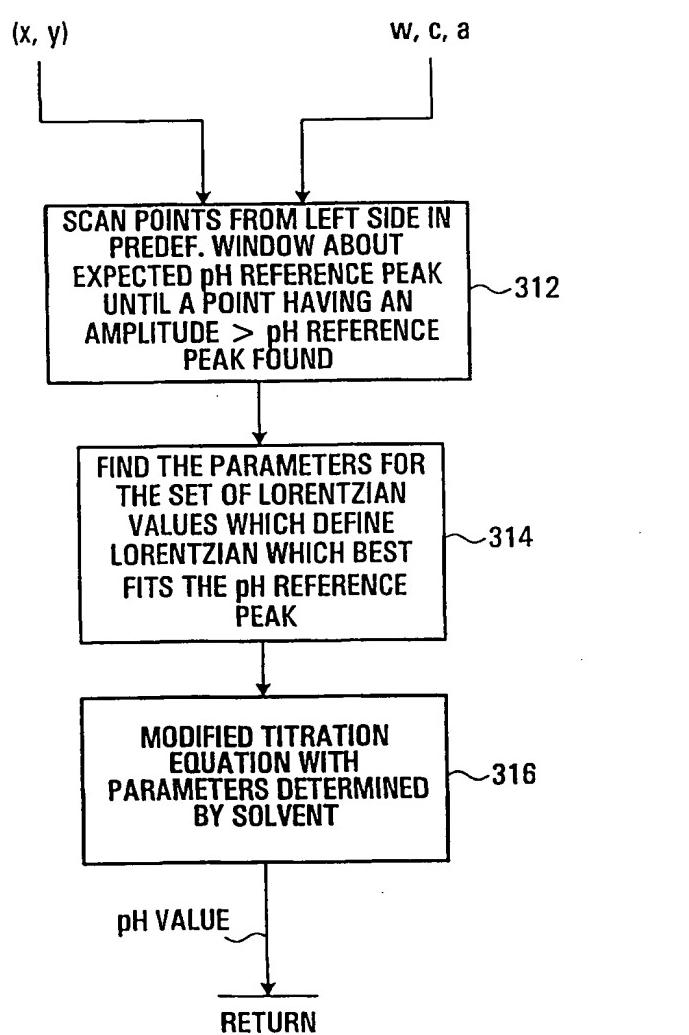


FIG. 11

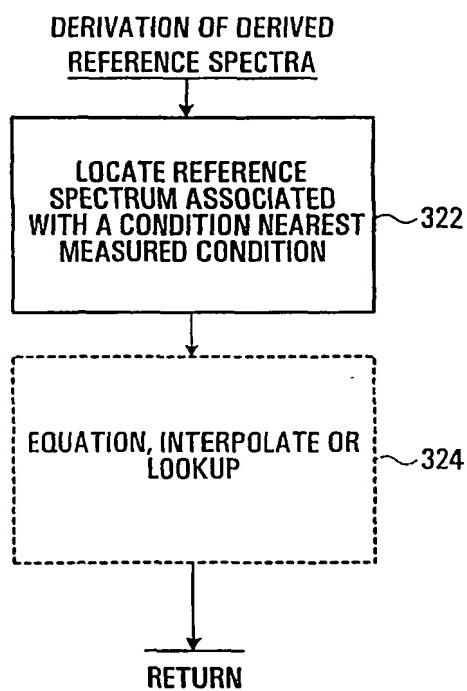


FIG. 12

Real Spectral Data - pH=5.45

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>1.318770</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 13A

```
<cluster>
  <protonNumber> 1 </protonNumber>
  <quantification> 0 </quantification>
  <subCluster>
    <centerPPM> 4.110990 </centerPPM>
    <lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
    <peak>
      <offsetCenterHz> -10.371092 </offsetCenterHz>
      <height> 0.054671 </height>
      <protonRatio> 0.124148 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> -3.448909 </offsetCenterHz>
      <height> 0.164509 </height>
      <protonRatio> 0.373572 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 3.456819 </offsetCenterHz>
      <height> 0.163879 </height>
      <protonRatio> 0.372141 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 10.371092 </offsetCenterHz>
      <height> 0.057309 </height>
      <protonRatio> 0.130139 </protonRatio>
    </peak>
  </subCluster>
</cluster>
</compound>
```

FIG. 13B

Interpolated Data - pH=5.28

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name> LacticAcid </name>
  <molecularWeight> 90.08 </molecularWeight>

  <experiment>
    <pH> 5.45 </pH>
    <temperatureKelvin> 298.150000 </temperatureKelvin> : copied
    <DSSRatio> 0.533668 </DSSRatio>
    <concentration> 4.308710 </concentration>
    <timestamp> Sept 5 2001 </timestamp>
    <sourceFID> lacticacid.fid </sourceFID> :copied
    <magnetMHz> 400.120699 </magnetMHz>
    <spectralWidthHz> 6006.006006 </spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber> 3 </protonNumber>
    <quantification> 1 </quantification>
    <subCluster>
      <centerPPM> 1.3202 </centerPPM> : interpolated
      <lorentzianWidthAdjust> 1.562004 </lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz> -3.453329 </offsetCenterHz>
        <height> 0.983656 </height>
        <protonRatio> 1.487641 </protonRatio>
      </peak>
      <peak>
        <offsetCenterHz> 3.453329 </offsetCenterHz>
        <height> 1.000000 </height>
        <protonRatio> 1.512359 </protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 14A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> 4.1149 </centerPPM> :interpolated
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 14B

Generic Lactic Acid record

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>y=m1(pH)+b1</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 15A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
<centerPPM> y=m2(pH)+b2 </centerPPM>
<lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
<peak>
<offsetCenterHz> -10.371092 </offsetCenterHz>
<height> 0.054671 </height>
<protonRatio> 0.124148 </protonRatio>
</peak>
<peak>
<offsetCenterHz> -3.448909 </offsetCenterHz>
<height> 0.164509 </height>
<protonRatio> 0.373572 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 3.456819 </offsetCenterHz>
<height> 0.163879 </height>
<protonRatio> 0.372141 </protonRatio>
</peak>
<peak>
<offsetCenterHz> 10.371092 </offsetCenterHz>
<height> 0.057309 </height>
<protonRatio> 0.130139 </protonRatio>
</peak>
</subCluster>
</cluster>
</compound>
```

FIG. 15B

Generic Lactic Acid record with Lookup Table link

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>LOOKUP TABLE LINK1</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 16A

```
<cluster>
<protonNumber> 1 </protonNumber>
<quantification> 0 </quantification>
<subCluster>
  <centerPPM> LOOKUP TABLE LINK2 </centerPPM>
  <lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
  <peak>
    <offsetCenterHz> -10.371092 </offsetCenterHz>
    <height> 0.054671 </height>
    <protonRatio> 0.124148 </protonRatio>
  </peak>
  <peak>
    <offsetCenterHz> -3.448909 </offsetCenterHz>
    <height> 0.164509 </height>
    <protonRatio> 0.373572 </protonRatio>
  </peak>
  <peak>
    <offsetCenterHz> 3.456819 </offsetCenterHz>
    <height> 0.163879 </height>
    <protonRatio> 0.372141 </protonRatio>
  </peak>
  <peak>
    <offsetCenterHz> 10.371092 </offsetCenterHz>
    <height> 0.057309 </height>
    <protonRatio> 0.130139 </protonRatio>
  </peak>
</subCluster>
</cluster>
</compound>
```

FIG. 16B

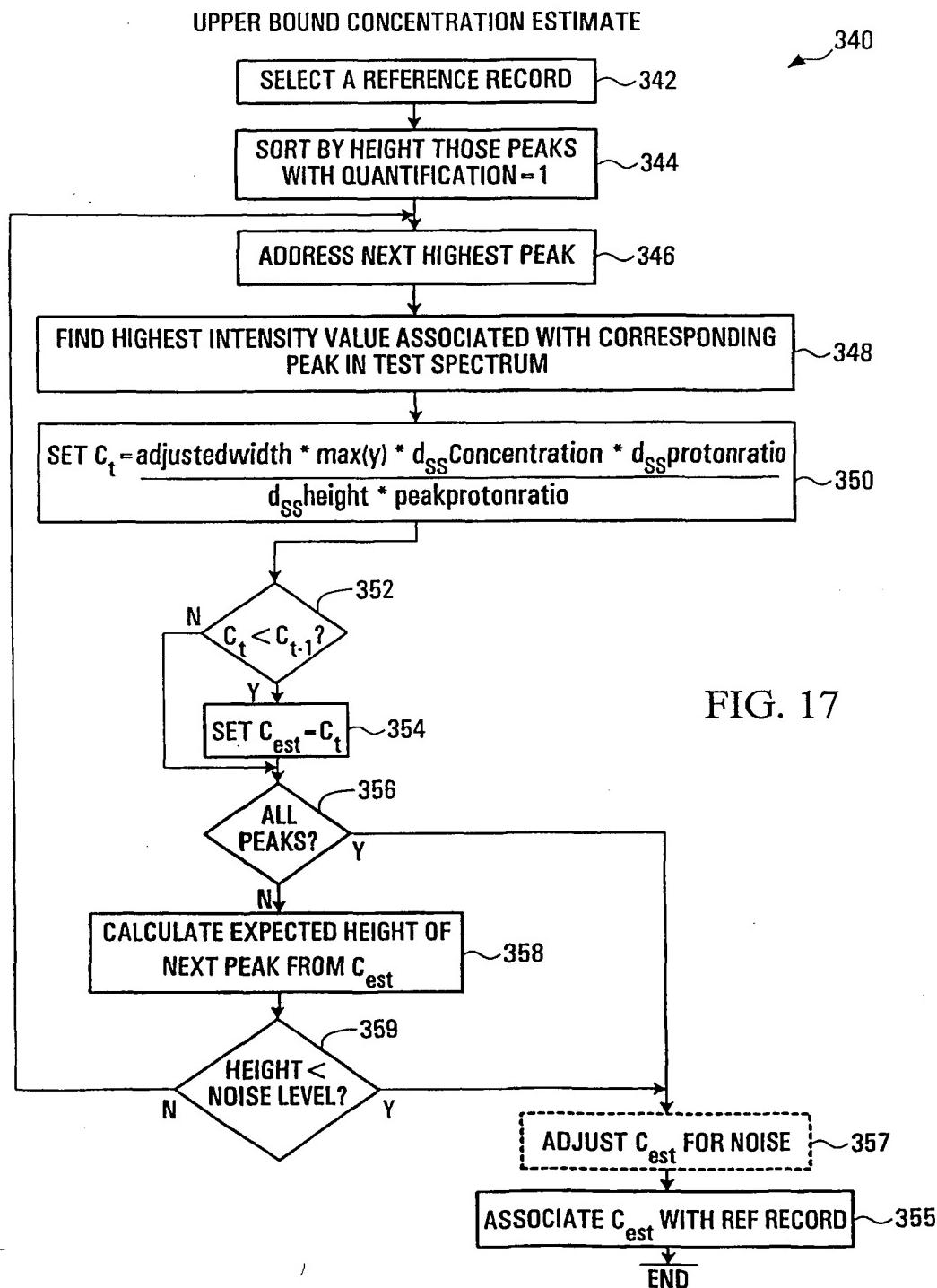


FIG. 17

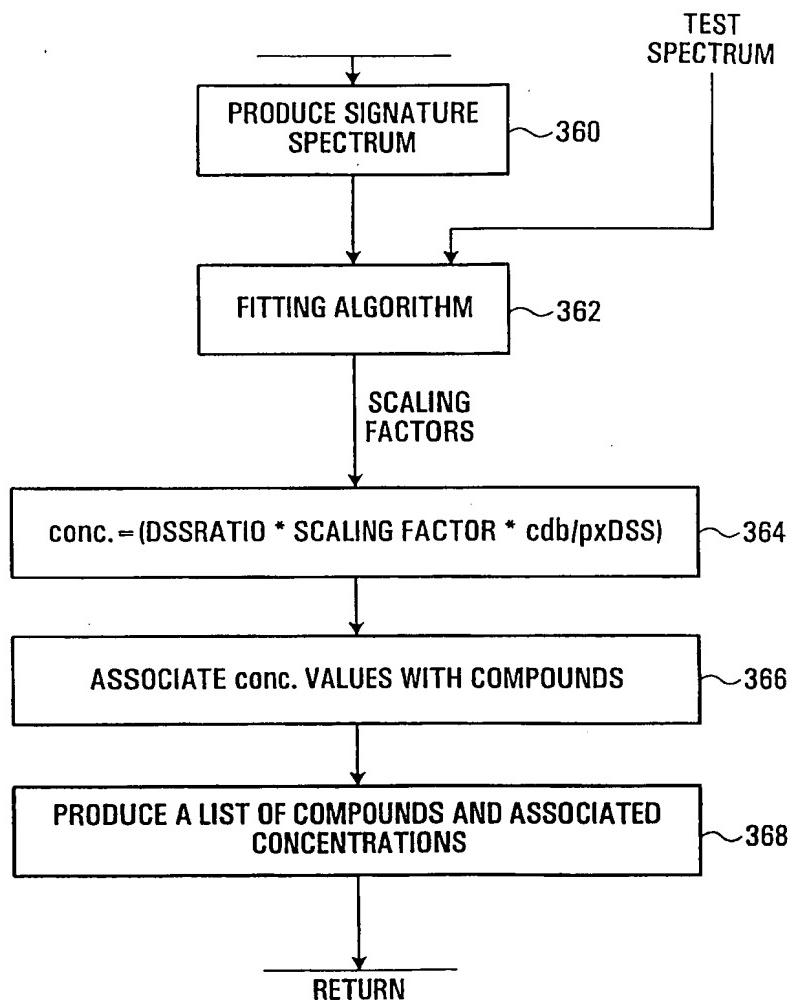


FIG. 18